

CLAIMS

1. A method for predicting pharmacokinetic properties of molecules comprising the steps of:
- 5 (a) preparing 2D-structures of molecules used as a training set;
- (b) constructing a 2D-fingerprint by counting the number of structural descriptors that potentially relate to a pharmacokinetic property, either manually or automatically using internally developed macro; wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures;
- 10 (c) analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and
- (d) calculating the pharmacokinetic property of a trial molecule using the above obtained QSPR model.
- 15 2. A method of Claim 1, wherein the pharmacokinetic property is absorption.
3. A method of Claim 1, wherein the pharmacokinetic property is distribution.
4. A method of Claim 1, wherein the pharmacokinetic property is metabolism.
5. A method of Claim 1, wherein the pharmacokinetic property is excretion.
6. A method of Claim 1, wherein the internally developed macro comprises the macro
- 20 script 2dfp.spl or 2dfp_abs.spl, written in SYBYL™ Programming Language (SPL).
7. A system for predicting pharmacokinetic properties of molecules comprising:
- (a) means for preparing 2D-structures of molecules used as a training set;
- (b) means for constructing a 2D-fingerprint by counting the number of structural descriptors that potentially relate to a pharmacokinetic property, wherein said structural
- 25 descriptors consist of predefined 20 to 80 atoms/fragments or substructures;
- (c) means for analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and
- (d) means for calculating the pharmacokinetic property of a trial molecule using the
- 30 above obtained QSPR model.

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